Guanidine, N,N'''-(iminodi-8,1-octanediyl)bis-

13516-27-3 | DTXSID7042015

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.02e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.45e-01

Confidence level: 7.52e-01

Nearest Neighbors from the Training Set

Image not found
Isoproturon
Measured: 1.20e-11
Predicted: 3.23e-11

Image not found
Terbuthylazine
Measured: 1.10e-11
Predicted: 1.23e-11

Image not found
Cycloate
Measured: 3.54e-11
Predicted: 2.98e-11

Image not found
Bornyl acetate
Measured: 1.39e-11
Predicted: 1.36e-11

Image not found
Decamethylcyclopentasiloxane
Measured: 1.55e-12
Predicted: 1.74e-12